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A Generalized Rule For Non-Commuting Operators in Extended Phase Space

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Abstract

A generalized quantum distribution function is introduced. The corresponding ordering rule for non-commuting operators is given in terms of a single parameter. The origin of this parameter is in the extended canonical transformations that guarantees the equivalence of different distribution functions obtained by assuming appropriate values for this parameter.

1 Introduction

The hamiltonian formulation of classical mechanics treats the generalized coordinates, q, and momenta, p, as independent variables and in a symmetric way. In quantization procedure, however, one chooses the q- or p-representation destroying the equal standing of the two variables. In his pioneering work, Wigner [1] proposed quantum distribution function in phase space keeping the symmetry of q and p and defined the expectation values of observables in the manner of classical statistical mechanics. Here, we use the extended phase space technique proposed by Sobouti and Nasiri [2] and the canonical transformations in this space to introduced a generalized quantum distribution function. It is known that for any distribution function there is an ordering rule of non-commuting operators. Thus, for generalized distribution function a generalized ordering rule is introduced, as well. Assuming appropriate values for the parameter involved, different distribution functions and their corresponding ordering rules can be obtained. The origin of these parameters is in the extended canonical transformations in the extended phase space.

The layout of the paper is as follows: In section 2, a brief review of the extended phase space formalism is presented. In section 3, the generalized distribution function is introduced. Section 4, is devoted to conclusions.

2 A Review of EPS formalism

A direct approach to quantum statistical mechanics is proposed by Sobouti and Nasiri [2], by extending the conventional phase space and by applying the canonical quantization procedure to the extended quantities in this space. Here, a brief review of this formalism is presented. For more details, the interested reader may consult Sobouti and Nasiri [2].

Let $\mathcal{L}^q(q,\dot{q})$ be a lagrangian specifying a system in q space. A trajectory of the system in this space is obtained by solving the Euler-Lagrange equations for $q(t)$,

$$\frac{d}{dt}\frac{\partial \mathcal{L}^q}{\partial \dot{q}} - \frac{\partial \mathcal{L}^q}{\partial q} = 0. \tag{1}$$

The derivative $\frac{\partial \mathcal{L}^q}{\partial \dot{q}}$ calculated on an actual trajectory, that is, on a solution of Eq. (1), is the momentum p conjugate to q . The same derivative calculated on a virtual orbit, not a solution of Eq. (1), exists. It may not, however, be interpreted as a canonical momentum. Let $H(p,q)$ be a function in phase space which is the hamiltonian of the system, whenever p and q are canonical pairs. It is related to $\mathcal{L}^q$ through the Legendre transformation,

$$H(\frac{\partial \mathcal{L}^q}{\partial \dot{q}}, q) = \dot{q}\frac{\partial \mathcal{L}^q}{\partial \dot{q}} - \mathcal{L}^q(q,\dot{q}). \tag{2}$$

For a given $\mathcal{L}^q$, Eq. (2) is an algebraic equation for H. One may, however, take a different point of view. For a given functional form of $H(p,q)$, Eq. (2) may be considered as a differential equation for $\mathcal{L}^q$. Its non unique solutions differ from one another by total time derivatives. One may also study the same system in the momentum space. Let $\mathcal{L}^p(p,\dot{p})$ be a lagrangian in p space. It is related to $H(p,q)$ as follows,

$$H(p, \frac{\partial \mathcal{L}^p}{\partial \dot{p}}) = -\dot{p}\frac{\partial \mathcal{L}^p}{\partial \dot{p}} + \mathcal{L}^p(p,\dot{p}). \tag{3}$$

Here the functional dependence of H on its argument is the same as in Eq. (2). In principle, Eq. (3) should be solvable for $\mathcal{L}^p$ up to an additive total time derivative term. Once $\mathcal{L}^p$ is known the actual trajectories in p space are obtainable from an Euler-Lagrange equation analogous to Eq. (1) in which q is replaced by p. That is

$$\frac{d}{dt}\frac{\partial \mathcal{L}^p}{\partial \dot{p}} - \frac{\partial \mathcal{L}^p}{\partial p} = 0. \tag{4}$$

The derivative $\frac{\partial \mathcal{L}^p}{\partial \dot{p}}$ along an actual p trajectory is the canonical coordinate conjugate to p . Calculated on a virtual orbit, it is not.

A formulation of quantum statistical mechanics is possible by extending the conventional phase space and by applying the canonical quantization procedure to the extended quantities in this space. Assuming the phase space coordinates p and q to be independent variables on the virtual trajectories, allows one to define momenta π_p and π_q, conjugate to p and q, respectively. One may combine the

two pictures and define an extended lagrangian in the phase space as the sum of p and q lagrangians,

$$\mathcal{L}(p,q,\dot{p},\dot{q}) = -\dot{p}q - \dot{q}p + \mathcal{L}^p(p,\dot{p}) + \mathcal{L}^q(q,\dot{q}). \tag{5}$$

The first two terms in Eq. (5) constitute a total time derivative. The equations of motion are

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{p}} - \frac{\partial \mathcal{L}}{\partial p} = \frac{d}{dt}\frac{\partial \mathcal{L}^p}{\partial \dot{p}} - \frac{\partial \mathcal{L}^p}{\partial p} = 0, \tag{6}$$

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} = \frac{d}{dt}\frac{\partial \mathcal{L}^q}{\partial \dot{q}} - \frac{\partial \mathcal{L}^q}{\partial q} = 0. \tag{7}$$

The p and q in Eqs. (5-7) are not, in general, canonical pairs. They are so only on actual trajectories and through a proper choice of the initial values. This gives the freedom of introducing a second set of canonical momenta for both p and q. One does this through the extended lagrangian. Thus

$$\pi_p = \frac{\partial \mathcal{L}}{\partial \dot{p}} = \frac{\partial \mathcal{L}^p}{\partial \dot{p}} - q, \tag{8}$$

$$\pi_q = \frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial \mathcal{L}^q}{\partial \dot{q}} - p. \tag{9}$$

Evidently, π_p and π_q vanish on actual trajectories and remain non zero on virtual ones. From these extended momenta, one defines an extended hamiltonian,

$$\begin{aligned}\mathcal{H}(\pi_p,\pi_q,p,q) &= \dot{p}\pi_p + \dot{q}\pi_q - \mathcal{L} = H(p+\pi_q,q) - H(p,q+\pi_p) \\ &= \sum \frac{1}{n!}\left\{\frac{\partial^n H}{\partial p^n}\pi_q^n - \frac{\partial^n H}{\partial q^n}\pi_p^n\right\}.\end{aligned} \tag{10}$$

Using the canonical quantization rule, the following postulates are outlined: a) Let p, q, π_p and π_q be operators in a Hilbert space, $\mathbf{X}$, of all square integrable complex functions, satisfying the following commutation relations

$$[\pi_q, q] = -i\hbar, \qquad \pi_q = -i\hbar\frac{\partial}{\partial q}, \tag{11}$$

$$[\pi_p, p] = -i\hbar, \qquad \pi_p = -i\hbar\frac{\partial}{\partial p}, \tag{12}$$

$$[p,q] = [\pi_p,\pi_q] = 0. \tag{13}$$

By virtue of Eqs. (11-13), the extended hamiltonian, $\mathcal{H}$, will also be an operator in $\mathbf{X}$. b) A state function $\chi(p,q,t) \in \mathbf{X}$ is assumed to satisfy the following dynamical equation

$$\begin{aligned}i\hbar\frac{\partial \chi}{\partial t} &= \mathcal{H}\chi = [H(p - i\hbar\frac{\partial}{\partial q}, q) - H(p, q - i\hbar\frac{\partial}{\partial p})]\chi \\ &= \sum \frac{(-i\hbar)^n}{n!}\left\{\frac{\partial^n H}{\partial p^n}\frac{\partial^n}{\partial q^n} - \frac{\partial^n H}{\partial q^n}\frac{\partial^n}{\partial p^n}\right\}\chi.\end{aligned} \tag{14}$$

c) The averaging rule for an observable $O(p,q)$, a c-number operator in this formalism, is given as

$$< O(p,q) >= \int O(p,q)\chi^*(p,q,t)dpdq. \tag{15}$$

To find the solutions for Eq. (14) one may assume

$$\chi(p,q,t) = F(p,q,t)e^{-ipq/\hbar} \tag{16}$$

The phase factor comes out due to the total derivative in the lagrangian of Eq. (5), -d(pq)/dt. The effect is the appearance of a phase factor, $exp(-ipq/\hbar)$, in the state function that would have been in the absence of the total derivative. It is easily verified that

$$(p - i\hbar\frac{\partial}{\partial q})\chi = i\hbar\frac{\partial F}{\partial q}e^{-ipz/\hbar} \tag{17}$$

$$(q - i\hbar\frac{\partial}{\partial p})\chi = i\hbar\frac{\partial F}{\partial p}e^{-ipz/\hbar} \tag{18}$$

Substituting Eqs. (17) and (18) in Eq. (14) and eliminating the exponential factor gives

$$H(-i\hbar\frac{\partial}{\partial q}, q) - H(p, -i\hbar\frac{\partial}{\partial p})F = i\hbar\frac{\partial F}{\partial t}. \tag{19}$$

Equation (19) has separable solutions of the from

$$F(p,q,t) = \psi(q,t)\phi^*(p,t), \tag{20}$$

where $\psi(q,t)$ and $\phi(p,t)$ are the solutions of the Schrodinger equation in q and p representations, respectively. The solution of the form (16) associated with anti-standard ordering rule satisfies Eq. (14) and is one possible distribution function. For more details on the admissibility of the distribution functions, their interesting properties and the correspondence rules, one may consult Sobouti and Nasiri [2].

3 Generalized distribution function and ordering rule

In 1932 Wigner [1] proposed the distribution

$$W(q,p) = \frac{1}{\pi\hbar}\int < q - y|\hat{\rho}|q + y > e^{ipy/\hbar}dy, \tag{21}$$

for a system in mixed state represented by a density matrix $\hat{\rho}$. The expectation value for an operator $\hat{O}$ calculated with $W(q,p)$ has the same value as ordinary quantum average with wave function ψ, i.e.

$$< \hat{O} >_\psi = \int W(q,p)O(q,p)dpdq, \tag{22}$$

where $O(q,p)$ is a classical function corresponding to operator $\hat{O}$ and is given according to wigner prescription by[3]

$$O(q,p) = \int < q - \frac{z}{2}|\hat{O}|q + \frac{z}{2} > e^{ipz/\hbar} dz. \tag{23}$$

Similarly, the distribution function of Eq. (16) could be written as

$$\chi(q,p) = \frac{1}{2\pi\hbar} \int < q|\hat{\rho}|q + z > e^{ipz/\hbar} dz, \tag{24}$$

and corresponding averaging rule

$$< \hat{O}(q,p) >_{\chi} = \int \chi(q,p) O(q,p) dp dq, \tag{25}$$

where the classical function $O(q,p)$ is given by

$$O(q,p) = \int < q|\hat{O}|q + z > e^{ipz/\hbar} dz. \tag{26}$$

Let a generalized distribution function be defined as

$$P_{\alpha}(q,p) = \frac{1}{2\pi\hbar} \int < q + \alpha z|\hat{\rho}|q + (\alpha + 1)z > e^{ipz/\hbar} dz, \tag{27}$$

and the corresponding ordering rule as

$$O_{\alpha}(q,p) = \int < q + \alpha z|\, \hat{O}|q + (\alpha + 1)z > e^{ipz/\hbar} dz, \tag{28}$$

where α is a parameter specifying the given distribution function, that is, for $\alpha = \frac{-1}{2}$ one has the Wigner function, for $\alpha = 0$ one has the standard distribution function and etc. The origin of α is in the canonical transformations in the extended phase space that serve to obtain the different distribution functions [2]. Equations (27)and (28) may be rewritten as

$$P_{\alpha}(q,p) = \frac{1}{2\pi\hbar} \int < q|e^{i\hat{p}\alpha z/\hbar} \hat{\rho} e^{-i\hat{p}\alpha z/\hbar}|q + z > e^{ipz/\hbar} dz, \tag{29}$$

$$O_{\alpha}(q,p) = \int < q|e^{i\hat{p}\alpha z/\hbar} \hat{O} e^{-i\hat{p}\alpha z/\hbar}|q + z > e^{ipz/\hbar} dz. \tag{30}$$

Equations (29) and (30) relate the generalized distribution function and the corresponding ordering rule to those of the (SN) representation by a unitary transformation. Thus, using the EPS representation as the basis, one may introduce different representations using Eqs. (29) and (30) for different values of α. As an example, consider an operator as $\hat{O} = \hat{q}^m \hat{p}^n$. Using Eq. (28) the classical function corresponding to this operator after a lengthy calculations becomes

$$O_{\alpha}(p,q) = \sum_{r=0}^{m} \binom{m}{r} \frac{n!}{(n-r)!} (i\hbar\alpha)^r p^{n-r} q^{m-r}, n \leq r. \tag{31}$$

Assuming $\alpha = \frac{-1}{2}$, Eq. (31) will be identical with that of Wyle-Wigner ordering rule [3], and for $\alpha = 0$, one obtains the standard ordering rule [4].

4 Conclusions

In the phase space approach to quantum mechanics each distribution function corresponds to an ordering rule. In this paper we introduce a generalized distribution function and corresponding generalized ordering rule. A parameter, α serves to specify the different quantum distribution functions. The origin of the parameter α comes from the extended canonical transformations in the extended phase space. The cases of SN and Wigner distribution functions are worked out as examples.

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